The use of Fourier-transform near and mid-infrared spectroscopy for sea salt quality characterization

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Introduction

The production of the traditional sea salt is an ancient, hand-labour and sustainable activity with benefits for the ecosystem and economy of the regions where this type of activity is carried out.

There are clear differences between flower of salt and traditional sea salt in terms of price and physico-chemical characteristics.

Fig. 1. Natural Park of 'Ria Formosa' (Algarve, Portugal)

The main objective of this work is to ascertain whether FT-MIR and NIR in combination with multivariate analysis have the capacity to discriminate sea salts with different geographical origins and physico-chemical characteristics.

Sampling and Analysis

Table 1. Information relative to the analysed sea salt samples.

Salt code	Type of salt	Origin	Class	Salt code	Type of salt	Origin	Class
F2	Flower of salt	Portugal	Non-commercial	A12	Salt	Portugal	Non-commercial
F4	Flower of salt	Portugal	Non-commercial	A13	Salt	Portugal	Non-commercial
F1	Flower of salt	Portugal	Commercial	A14	Salt	Portugal	Non-commercial
F6	Flower of salt	Portugal	Commercial	A15	Salt	Portugal	Non-commercial
F7	Flower of salt	Portugal	Commercial	A17	Salt	Portugal	Commercial
F8	Flower of salt	Portugal	Commercial	A19	Salt	Portugal	Commercial
F9	Flower of salt	Portugal	Commercial	A20	Salt	Portugal	Commercial
F11	Flower of salt	Portugal	Commercial	A27	Salt	France	Non-commercial
F12	Flower of salt	Portugal	Commercial	A18	Salt	France	Commercial
F3	Flower of salt	France	Non-commercial	A16	Salt	Spain	Commercial
F10	Flower of salt	Spain	Commercial	A21	Salt	Spain	Commercial
A11	Salt	Portugal	Non-commercial	A24	Salt	Spain	Commercial

Fig. 2. Map with sea salt origins

Fig. 3. Sea salt pans (Aveiro, Portugal)

Fig. 4. Mid-infrared-ATR spectrometer (Perkin-Elmer)

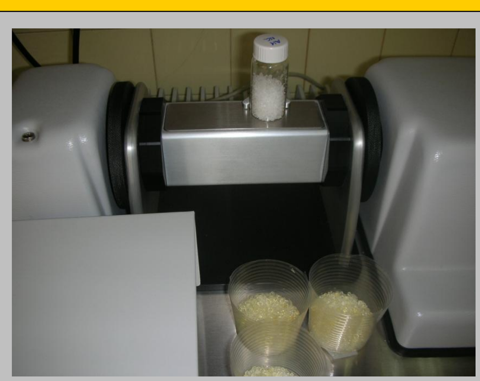

Fig. 5. Near-infrared spectrometer (ABB Bomem)

- ❑ Calcium and magnesium were determined by atomic absorption spectrometry and potassium by flame emission photometry.
- ❑ Analysis were performed using Matlab V.6.5 (MathWorks, USA)

Results

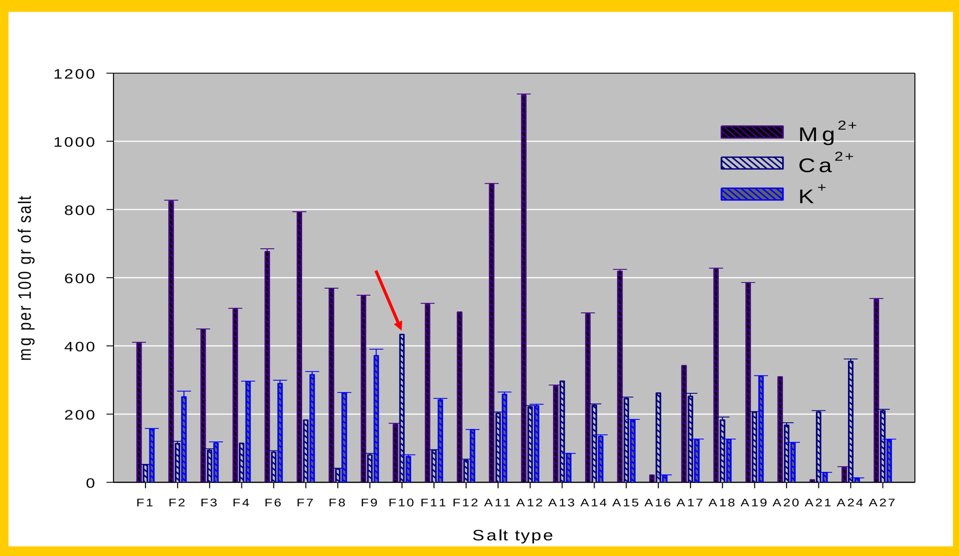

Fig. 6. Total concentration of Mg^{2+}, Ca^{2+} and K^+ in sea salt samples by atomic absorption spectrometry. The bars represents average values (n=3) ± SD

- The atomic absorption results show that **traditional sea salt samples have higher levels of Ca^{2+}** than flower of salt samples (Fig. 6). An unexpected **high concentration of Ca^{2+} was detected in a flower of salt coded as 'F10'**.
- The sample **'F10' is a commercial sample** from Spain (Table 1).

Results

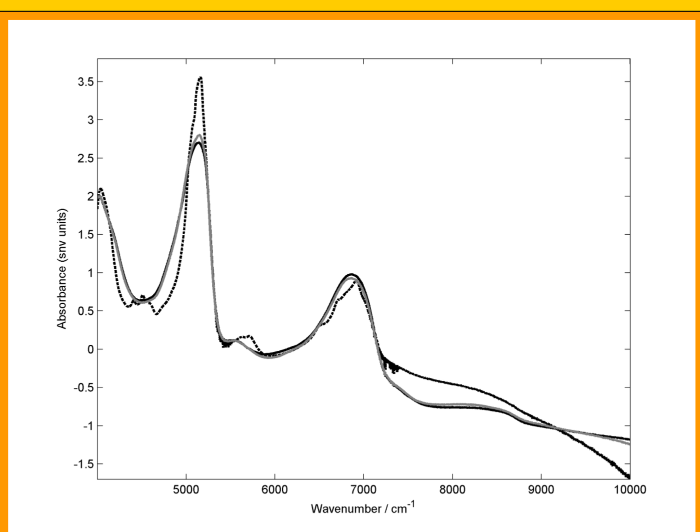

Fig. 7. Typical average NIR spectrum features of sea salt samples from Spain (dashed trace), Portugal (dark trace) and France (light trace).

❖ By visual inspection of the NIR spectrum it was evident that samples from Spain have a very distinct pattern in several spectral regions (Fig.7).

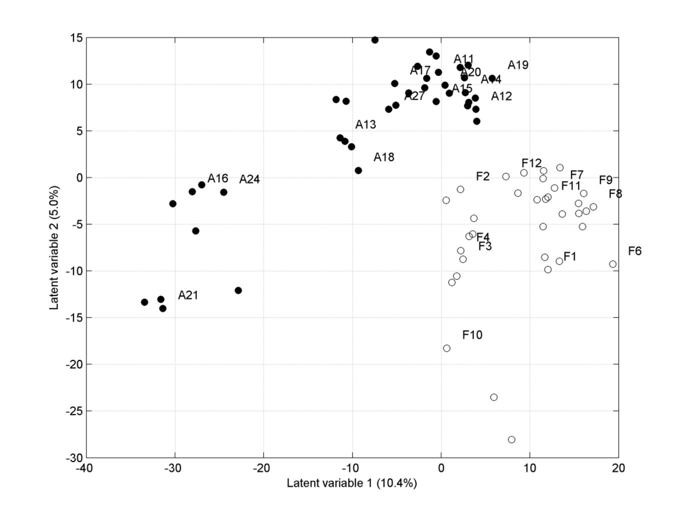

Fig. 8. PCA of single NIR sea salts spectra. Black circles (●) represent traditional sea salt and white circles (○) represent flower of salt.

❖ PCA analysis shows a discrimination between sea salt types in the spectral region between 7500-10000 cm^{-1} (Fig.8) .

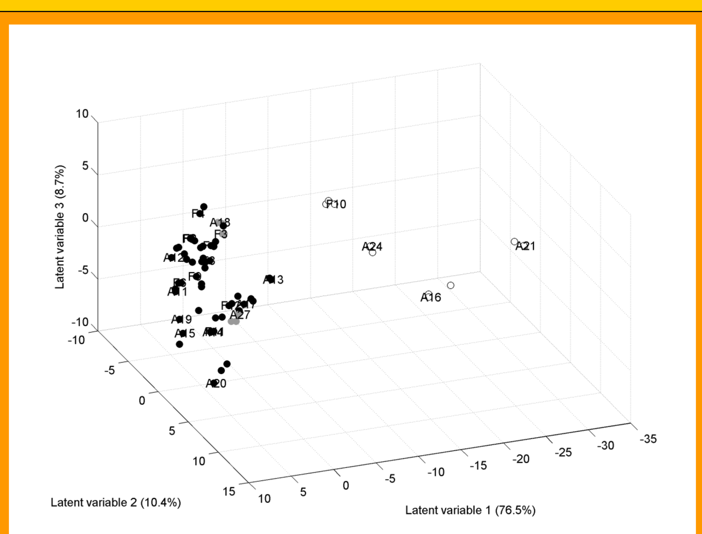

Fig. 9. PCA of single NIR sea salts spectra. Black (●) and grey circles (○) represent Atlantic sea salts (Portugal and France) and white circles (○) represents salts from Spain.

❖ The NIR spectrum also allows discrimination between Mediterranean (Spanish) from Atlantic (Portugal and France) salts using the spectral region between 7500-10000 cm^{-1} (Fig.9).

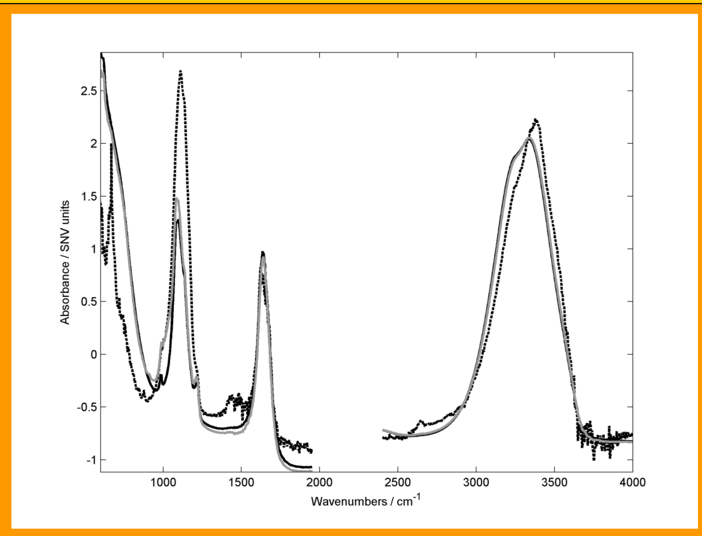

Fig. 10. Typical average MIR spectrum features of sea salt samples from Spain (dashed trace), Portugal (dark trace) and France (light trace).

❖ It was observed that in the spectrum region between 950 and 1250 cm^{-1} a series of bands of different intensity arise 90,1005. 1080, 1100, 1140, 1220 cm-1 (Figs. 10 and 11).

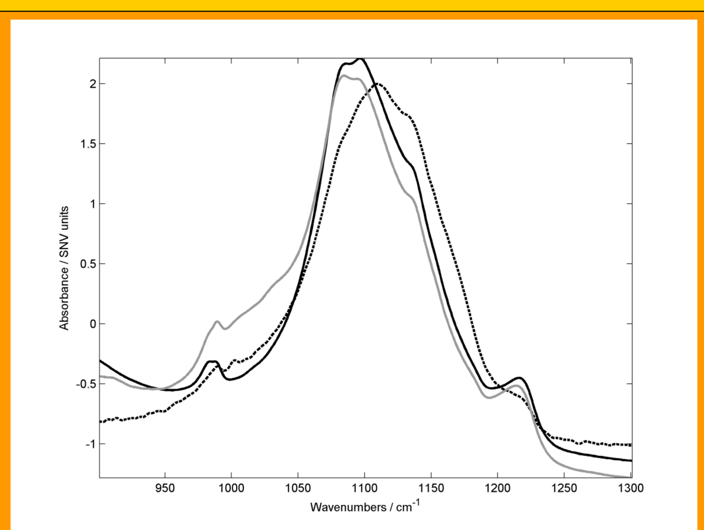

Fig. 11. Typical average MIR spectrum features (950-1250 cm-1) of sea salt samples from Spain (dashed trace), Portugal (dark trace) and France (light trace).

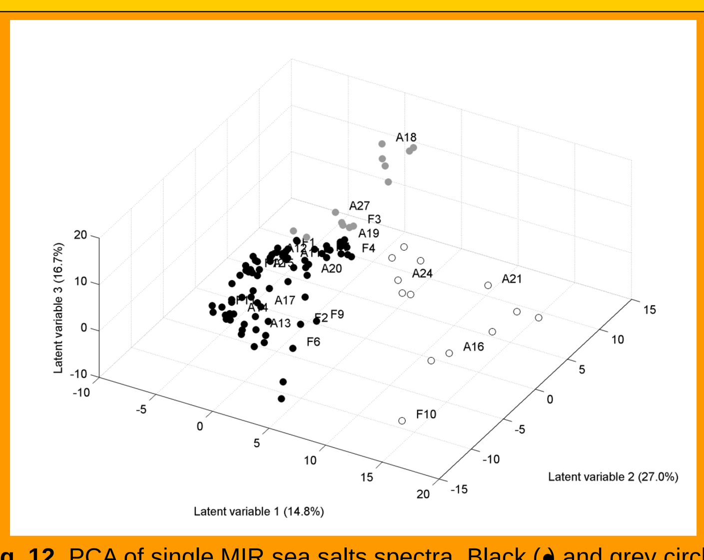

Fig. 12. PCA of single MIR sea salts spectra. Black (●) and grey circles (○) represent Atlantic sea salts (Portugal and France) and white circles (○) represents salts from Spain.

❖ The MIR spectrum allows discrimination of sea salts according geographical origin using the spectral region between 950-1250 cm^{-1} (Fig.12).

Conclusions:

- ➢ Both NIR and MIR are adequate techniques for characterization of sea salts in a straightforward way.
- ➢ For building regression models for field application or extending the scope of the models (e.g., identifying other salt origins), a higher number of samples should be included.
- ➢ The application of these techniques for sea salt can be used for the identification of counterfeit or adulterated salts or for manufacturers internal quality control.

Acknowledgements

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